The Stability of $RbAlSi_3O_8$ Under High Pressure Conditions

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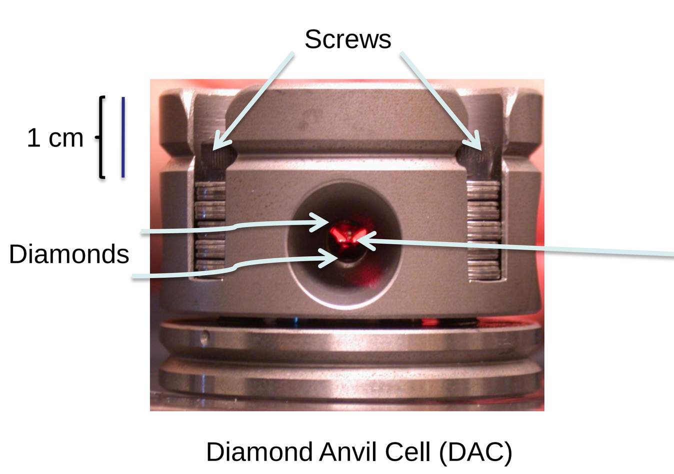
I Abstract

Potassium and Rubidium are minor and trace elements of the Earth's mantle, both of which have long-lived radioactive isotopes. ^{40}K is a significant energy source that contributes to the convection of the mantle and outer core, while ^{87}Rb is a geochemical tracer for long-lived mantle processes. In the Earth's crust, K and Rb are stored in feldspar, $KAlSi_3O_8$, the most abundant mineral in the crust. The mineral host of K and Rb in the mantle is uncertain, with implications on reactivity of alkali metals with the Earth's core. Sample preparation consisted of compressing $RbAlSi_3O_8$, Rubidium microcline (rubicline), under pressures of ~15 GPa (gigapascals) in a laser-heated diamond anvil cell (LHDAC). Synchrotron-based x-ray diffraction gives the structure and density at high pressures. The high-pressure structure of Rubidium microcline is similar to that of the high-pressure structure of feldspar, transforming to the hollandite structure at ~15 GPa, then to the hollandite II structure at ~25 GPa. Preliminary results yield the bulk modulus of Rubidium hollandite to be 210 (±10) GPa.

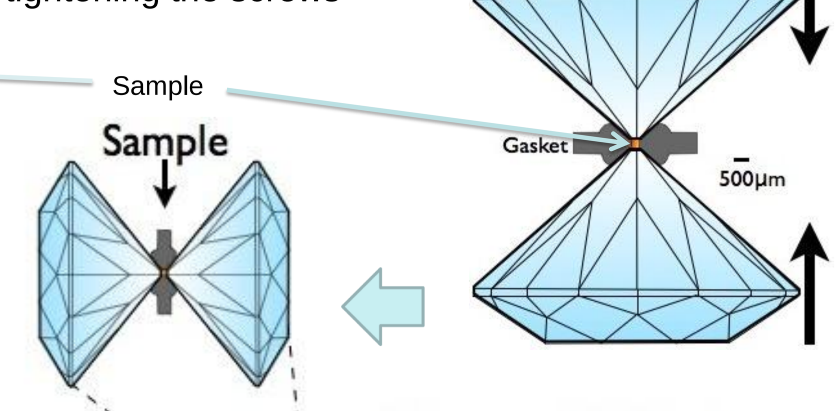
II Data Collection and Analysis

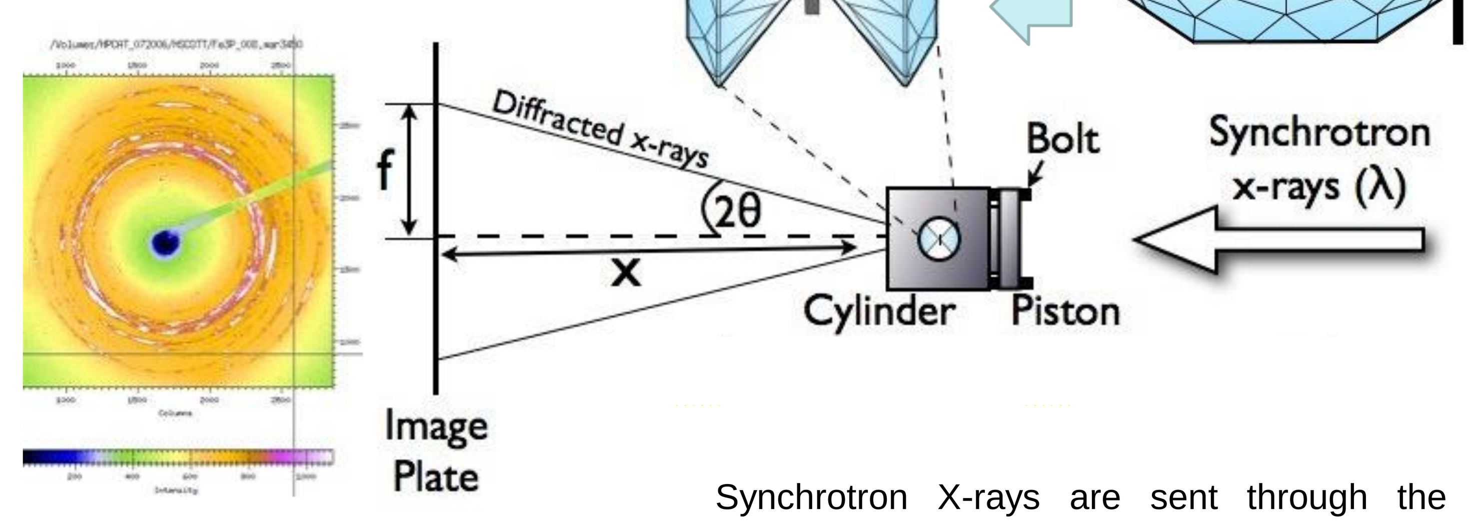
A sample is ground up and loaded into a diamond anvil cell between two diamonds

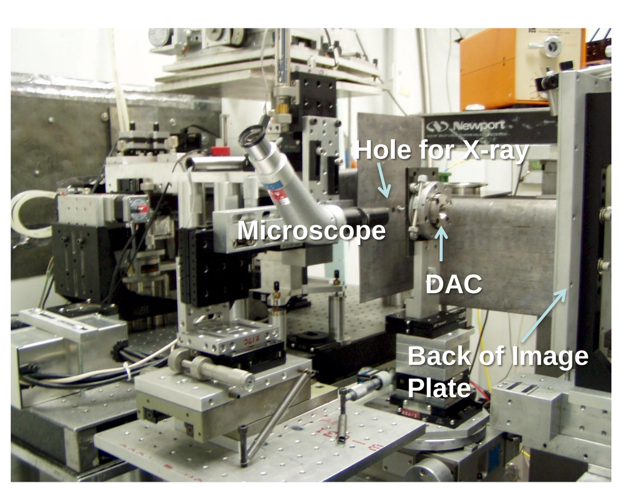


Diamond Anvil Cell (DAC)

Pressure is added onto the sample by tightening the screws







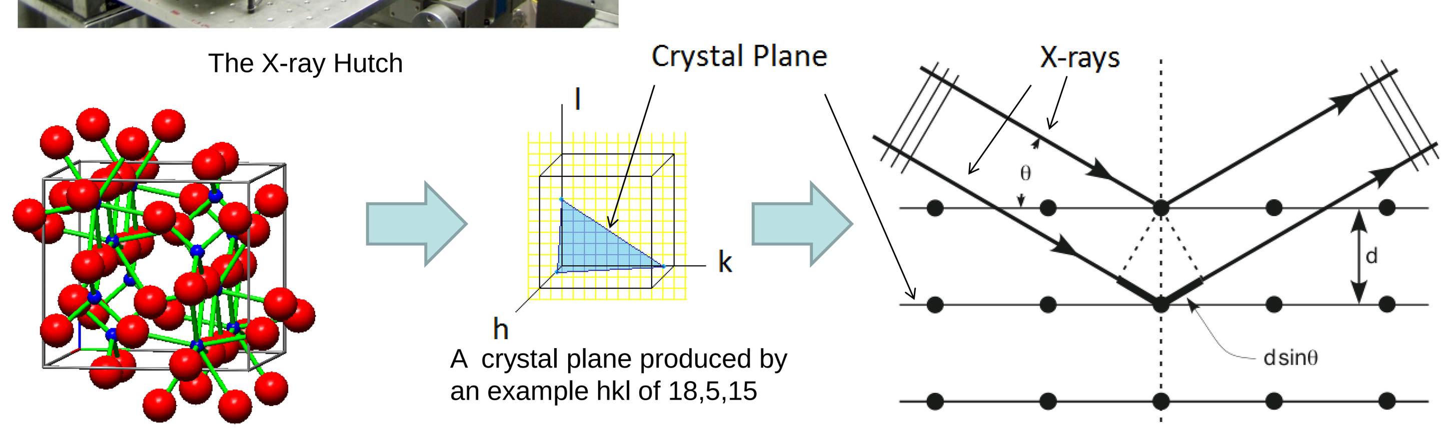
The X-ray Hutch

Synchrotron X-rays are sent through the diamonds and into the sample. The diffraction pattern is recorded on a digital image plate and integrated to create a one dimensional profile. The d-spacings (d) are determined from using Bragg's equation.

Bragg Diffraction:

$$\lambda = 2d\sin\theta$$

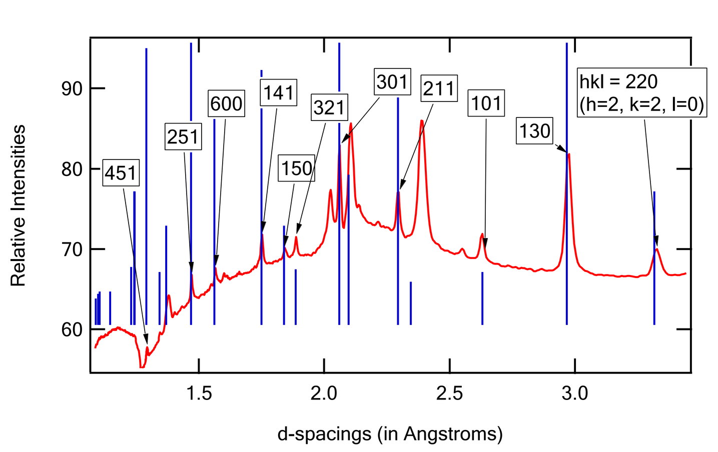
$$\tan 2\theta = \frac{f}{x}$$



Example Unit Cell

A crystal plane produced by an example hkl of 18,5,15

An "hkl" provides a set of "coordinates" along the x, y and z axes of a unit cell that define a crystal plane from which X-rays can diffract



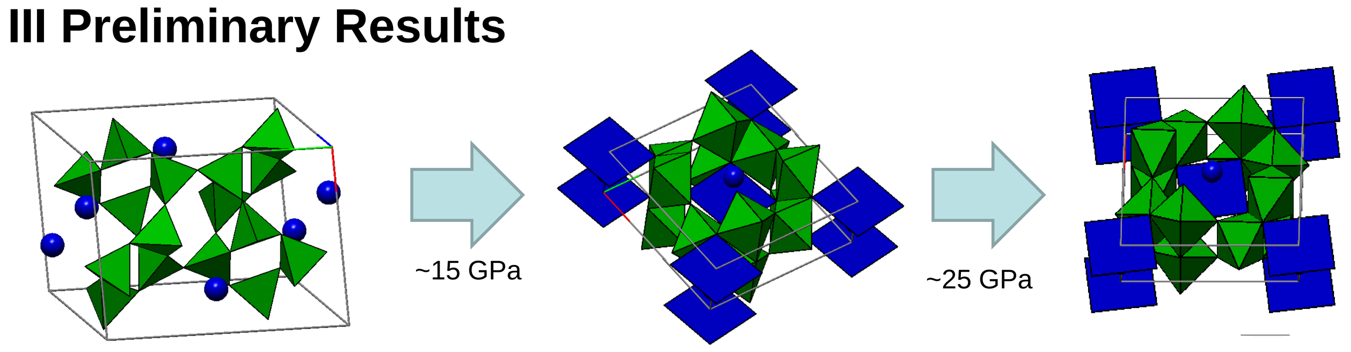
For each profile, as many peaks as possible are picked and assigned to an hkl

The d-spacings and hkl's for each peak are used to calculate the lattices, and sometimes the angles between the lattices

$$\frac{1}{d^2} = \frac{h^2+k^2}{a^2} + \frac{l^2}{c^2}$$

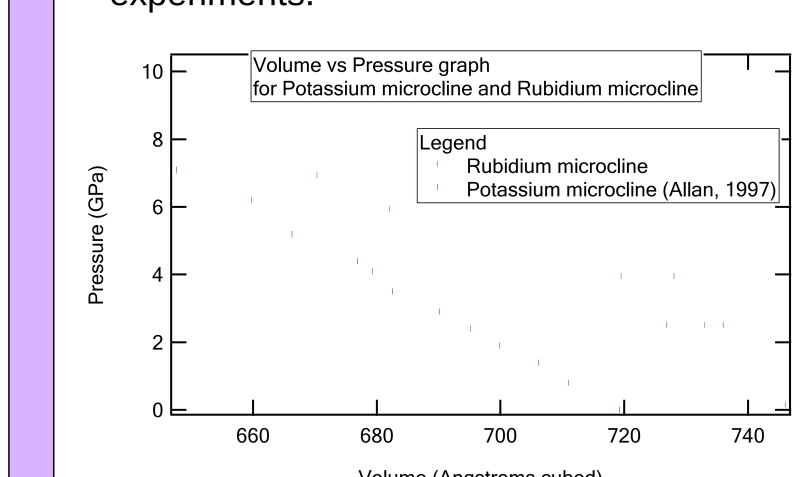
Equation for tetragonal crystal structures, used to find the lattices (a and c) of Rubidium hollandite

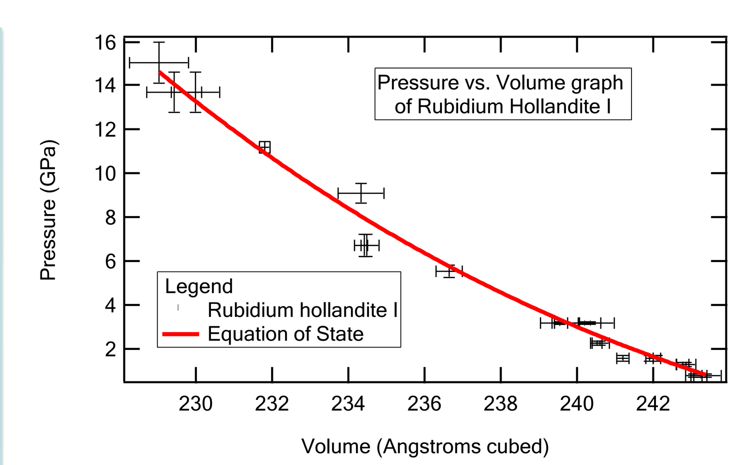
III Preliminary Results



Rubidium microcline — Rubidium hollandite — Rubidium hollandite II (inferred from Hirao, 2008)

Rubidium microcline goes through a phase transition into Rubidium hollandite at high temperatures and pressures. The hollandite structure is metastable to ambient pressure, allowing for a detailed equation of state measurement at pressures of 0-15 GPa. A sample synthesized at ~15 GPa and ~2500 K was reloaded in the diamond anvil cell with silicon oil for a quasi-hydrostatic pressure medium. The hollandite II structure is not quenchable to ambient pressure, and therefore the equation of state can only be inferred from synthesis experiments.



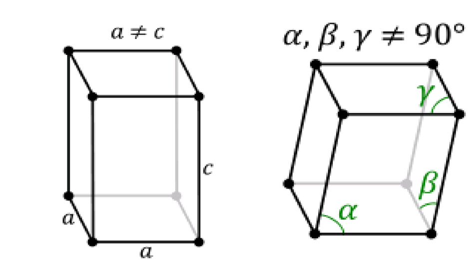


The bulk modulus (B_0) of Rubidium hollandite is 210 (±10) GPa, showing that Rubidium hollandite is less compressible than Potassium hollandite (B_0 = 180 GPa). B_0' is fixed to 4.

Analysis of Rubidium microcline is in progress.

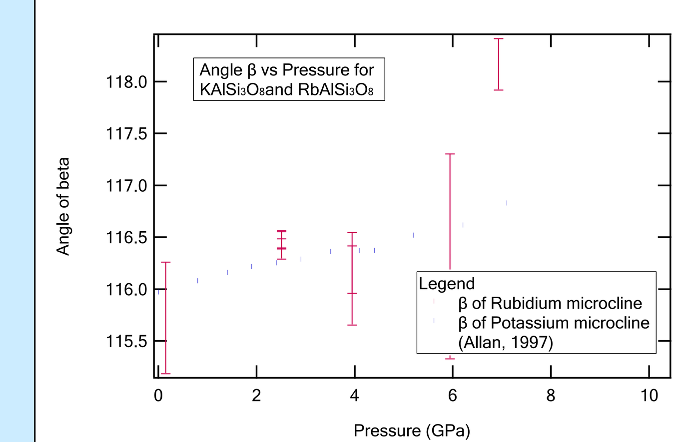
IV Discussion

• Unlike Rubidium hollandite, which has a tetragonal crystal structure, Rubidium microcline is triclinic, giving us six variables to solve for (lattices *a*, *b* and *c*; angles α, β and γ) instead of two (lattices *a* and *c* as in the case of hollandite) for every pressure state, allowing for a number of complications.



$$\frac{1}{d^2} = \frac{1}{Volume^2}\left(b^2c^2(\sin^2\alpha)h^2 + a^2c^2(\sin^2\beta)l^2 + a^2b^2(\sin^2\gamma)k^2 + 2abc^2(\cos\alpha\cos\beta - \cos\gamma)hk + 2a^2bc(\cos\beta\cos\gamma - \cos\alpha)kl + 2ab^2c(\cos\gamma\cos\alpha - \cos\beta)hl\right)$$

Equation for triclinic crystal structures, used to find the angles and lattice parameters for Rubidium microcline



• In the case of Potassium microcline, the peaks of the X-ray diffraction data were observed to be sensitive to the change of the β angle (Allan, 1997). Assuming the behavior of the β angle of Rubidium microcline to be similar to that of Potassium microcline might produce more satisfactory results.

• The difficulty in picking out and assigning peaks to hkl's for the diffraction data of Rubidium microcline rubicline may be due to coarsely powdered samples.

•Analyses indicate that Rubidium is capable of being stored in deep mantle conditions, which would constrain the age of the Earth's core. The similarity in observed phases between Potassium and Rubidium implies that these elements might be stored together in minor mineral phases in the Earth's mantle.

V Future Expectations and Goals

• Add more X-ray diffraction data to the existing Rubidium hollandite data for higher pressures to help better constrain the bulk modulus

• Find the temperatures and pressures where phase transitions take place between Rubidium microcline, Rubidium hollandite I and II

• Find the exact change in angles and lattice parameters with change of pressure for Rubidium hollandite II

• Do more X-ray diffraction experiments for Rubidium microcline with finer powdered samples

• Do similar analyses for $KAlSi_3O_8$

VI References

• Hirao, N., E. Ohtani, T. Kondo, T. Sakai and T. Kikegawa (2008), Hollandite II phase in $KAlSi_3O_8$ as a potential host mineral of potassium in the Earth's lower mantle, *Physics of the Earth and Planetary Interiors,* 166, 97-104

• Allan, D. R., and Angel, R. J. (1997), A high-pressure structural study of microcline ($KAlSi_3O_8$) to 7 GPa, *Eur. J. Mineral,* 9, 263-275